Journal of Chemical Health Risks

www.jchr.org

JCHR (2024) 14(4), 293-2098 | ISSN:2251-6727

Synthesis, Characterization and Optical properties of Pure and Nd-doped $BiFeO_3$ for Environmental Applications

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(Received: 11 June 2024 Revised: 16 July 2024 Accepted: 10 August 2024)

KEYWORDS

Photocatalytic Performance, Nanoparticles, X-r diffraction (XR UV-visible spect Band gap,

ABSTRACT:

For the environmental remediation and degradation of pollutants the study of advanced materials is rapidly increasing due to large varieties of application. $BiFeO_3$ (BFO) having a perovskite nano material with a rhombohedral R_3C space group showing tremendous attention in photo degradation of dyes. Photocatalytic activity of BFO nanoparticles is a favourable field of research in photocatalysis. Photocatalyst properties of BFO enhanced by doping because of its reduce band gap energy (2.0-2.77 eV), multiferroic property, strong photo absorption and crystal structure. Recently, researcher shows great interest in the photocatalytic and multiferroic properties and doping effects of $BiFeO_3$ (BFO). Nd-doped bismuth ferrite nanoparticles having general formula $Bi_{1-x}Nd_xFeO_3$ (x=0, 0.05, 0.10, 0.15, 0.20). Calcinations processes had done at two different temperature 550°C and 650°C. The size of nanoparticles is decreased by increasing the concentration of neodymium in the structure of BFO. The presence of neodymium (Nd) doped in BFO enhances the photocatalytic performance by reduction of the electron-hole pair recombination sites and reformation of the band gap to improve the visible light absorption. The X- ray diffraction studies show that on increasing the doping concentration on Bi-site there are gradual shift in the position of the X- ray diffraction peaks. The UV- visible spectra shows a gradual decrease in the band gap from 2.23 eV to 1.98 eV. The presence of neodymium (Nd) doped in BFO enhances the photocatalytic performance by reduction of the electron-hole pair recombination sites and reformation of the band gap to improve the visible light absorption.

Introduction:

Bismuth ferrite ($BiFeO_3$) is a multiferroic material that exhibits both ferroelectric and ferromagnetic behavior. It has attracted a lot of attention due to its potential applications in various fields such as sensors, photocatalysts, and photovoltaic cells, among others. However, there are some challenges that need to be overcome in order to fully realize the potential of bismuth ferrite in these applications. For example, one of the main challenges is that it has a relatively weak ferroelectric polarization compared to other ferroelectric materials, which can limit its performance in certain applications. Additionally, there are also concerns about the reliability and magnetization of bismuth ferrite, which can impact its potential use in certain applications. Despite these challenges, research on bismuth ferrite and its potential applications is ongoing, and there have been many advances in recent years in understanding the properties and behavior of this material. The band gap of BFO is an important parameter that determines its optical properties and can be modified by substituting ions in the material. One approach to modifying the properties of BFO is to substitute ions such as Bi$^+$ or Fe^{+3} with other metal ions, such as Nd. This can help to suppress the spatial non-uniformity of the magnetic structure in BFO, which has been reported by several researchers. However, there is limited information available on the effect of Nd substitution on the optical properties of BFO, particularly when synthesized using the sol-gel method. In this research, the aim is to study the optical properties of Nd-doped BFO nanoparticles synthesized using the sol-gel method, with the goal of understanding their potential use in the degradation of organic pollutants. The crystallographic and optical properties of these nanoparticles will be characterized using techniques such as X-ray diffraction (XRD) and UV-visible spectrophotometry [1-2].

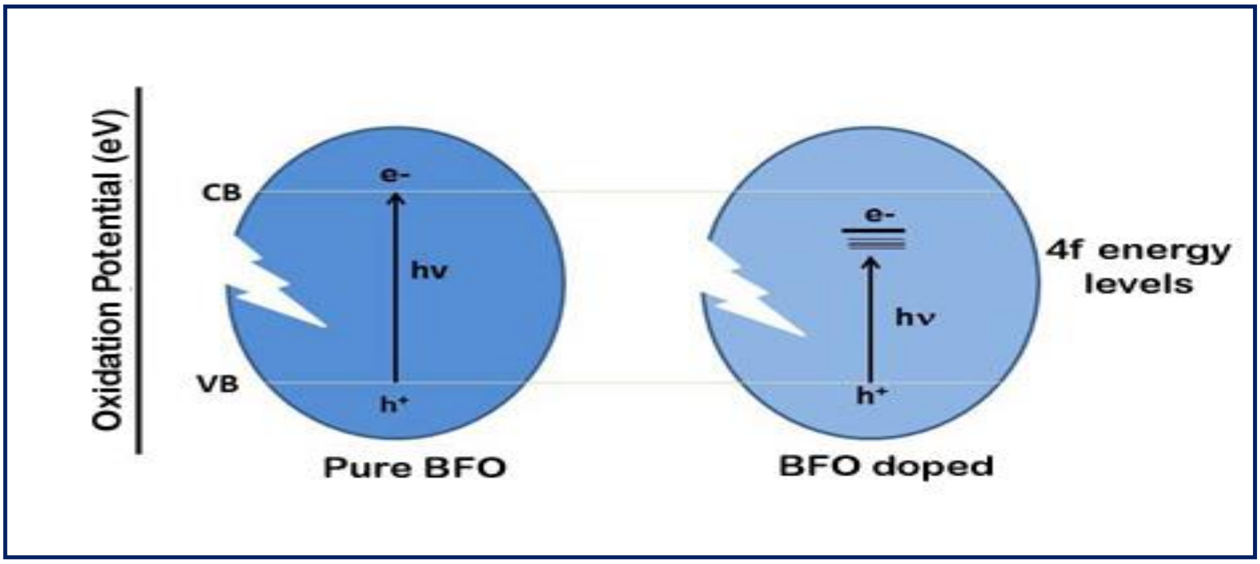

Fig.1: Schematic diagram showing band gap of BFO nanoparticles before and after doping

1. Materials and Methods:

A. Synthesis method for Nd-doped-$BiFeO_3$ Nanoparticle by Sol-Gel Method:

For synthesis of Nd-doped-BFO nanostructure, having general formula $Bi_{1-x}Nd_xFeO_3$ (BNFO) ($x = 0.05, 0.07, 0.10, 0.15, 0.20$) by Sol-Gel method. Bismuth nitrates $Bi\ (NO_3)_3.5H_2O$, ferric nitrate $Fe(NO_3)_3.9H_2O$ and Neodymium nitrate [$Nd(NO_3)_3$.6H2O], are used as metal source and propylene glycols are used as chelating agent. Addition of chelating agent chelation reaction starts which facilitate the gelation process. The chelating agents effect the phase and morphology of final product, which is controlled by molecular structure of the chelating agents. Chelating agent is added under constant stirring and heating at about 100ºC. After 2–3-hour liquid changes to fluffy gel which gives a brown-coloured fine $BiFeO_3$ nanoparticles. The as-prepared bismuth ferrite is calcined at 400-550ºC for 2-3 hour to obtained the $BiFeO_3$ nanoparticle. In process of calcinations the volatile matters were removed and finally get the pure phase of the $BiFeO_3$ nanoparticle and Pr-doped bismuth nitrate (BNFO) nanoparticles. [3-5]

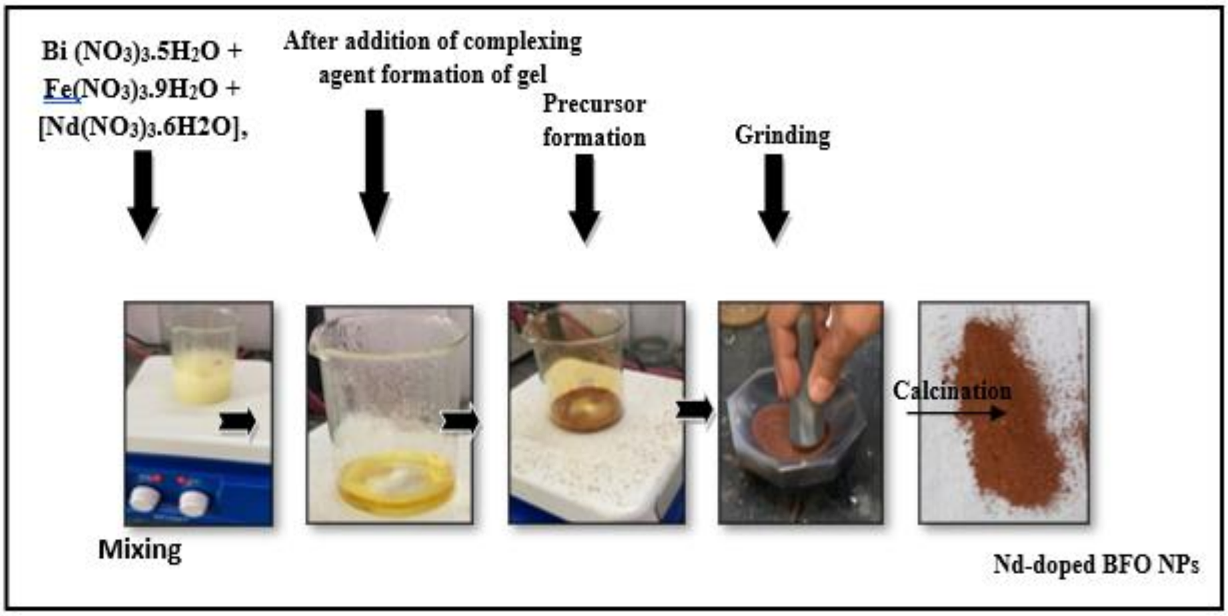

Fig.2: Schematic representation of synthesis of Nd doped $BiFeO_3$ NPs (doping with 5%, 7%, 10%, 15% and 20% Nd,)

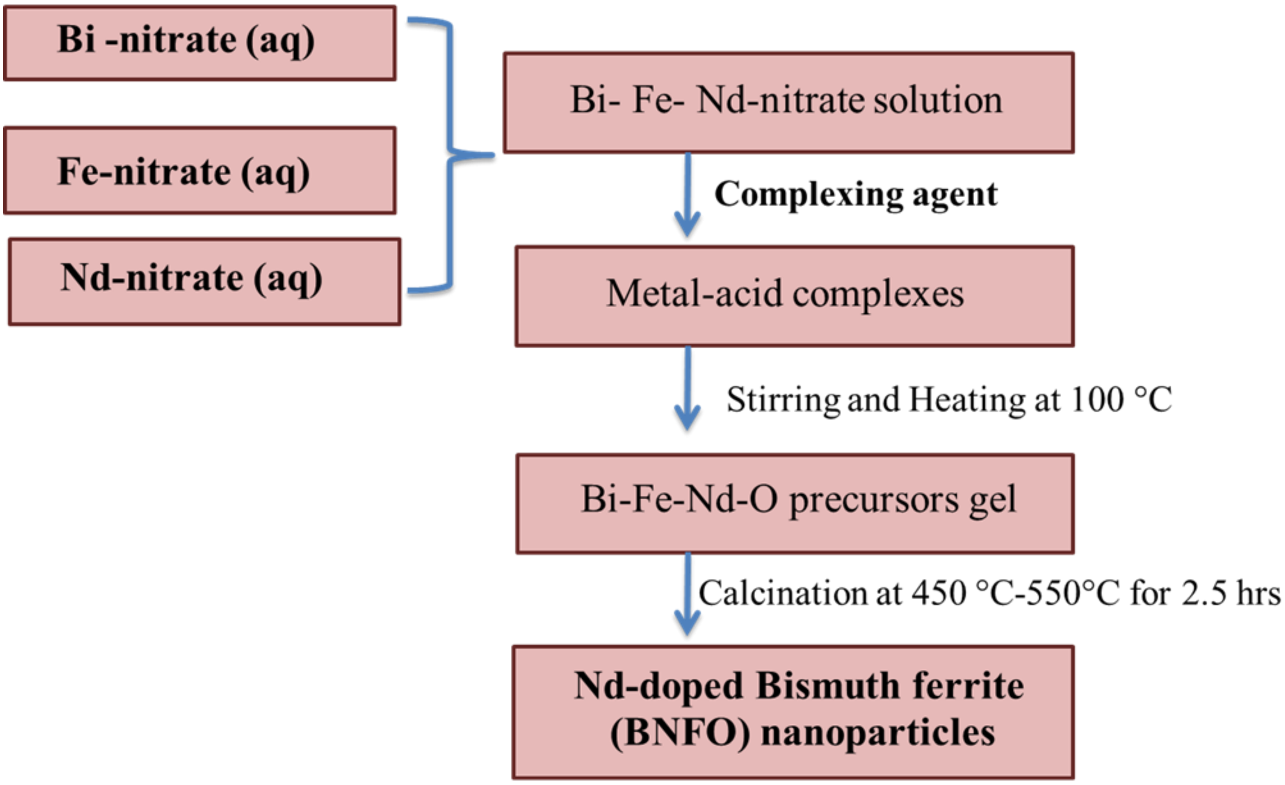

Fig.3: Flow diagram for the synthesis of Nd-doped $BiFeO_3$ nanoparticles

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2. Results and Discussion

A. X-ray Diffraction (XRD)

The size of nanoparticles is decreased by increasing the concentration of doping agent (Pr) in the structure of BFO. The X- ray diffraction studies show that on increasing the doping concentration of Pr on Bi-site there are gradual shift in the positions of the X- ray diffraction peaks. The prominent peaks in the XRD plots are confirming the synthesis of pure phase Bismuth Iron Oxide. The Debye-Scherer formula is commonly used to estimate the average grain size of nanocrystalline materials from their XRD patterns. The average grain size (D) was calculated using the formula the Full Width at Half Maxima (FWHM) of the high intense peak from XRD data. Sherre's Formula is very useful to predict the crystalline size of nanoparticles of nano size materials. [6-7]

The Formula is, $D = \frac{K\lambda}{\beta Cos\theta}$

Where, D = Size of crystallite, K = Scherre's constant, □ = Wavelength of X-Ray□ = Full width at half maximum □ = Peak position or Bragg angle in degrees.

B. UV-Vis Analysis of Optical properties:

$BiFeO_3$ (BFO) is a well-known photocatalyst material due to its unique optical and electronic properties. Neodymium (Nd) doping in BFO can result in $Bi_{1-x}Nd_xFeO_3$ (BNFO) particles, which have been shown to have improved photocatalytic properties due to changes in their structural and optical properties. Measuring the transmission spectra of BNFO particles in the 200-2500 nm range can reveal changes in the material's optical properties as the Nd doping concentration increases. The decrease in transmittance and increase in refractive index with increasing Nd doping concentration is thought to be due to an increase in structural disorder in the BNFO particles. The increase in structural disorder is caused by the substitution of Nd ions for Bi ions in the BFO lattice, which can result in strain and defects in the material. The decrease in the optical band gap energy of Nd-doped BNFO particles in comparison to pure BFO is also an important property for photocatalysis. Lower band gap energy means that the material can absorb a wider range of light, making it more efficient at converting light energy into chemical energy for the degradation of organic pollutants and dyes.

The observed photocatalytic activity of Nd-doped BNFO particles when tested using dyes such as methylene blue and Rhodamine-B confirms that the material is a suitable candidate for photocatalysis. The high refractive index and lower band gap energy of Nd-doped BNFO makes it a promising material for use in various photocatalytic applications such as water purification, air purification, and the degradation of hazardous organic compounds. However, the final photocatalytic activity depends on many factors including light source, atmosphere, and reaction conditions. It is also non-toxicity and inexpensive cost-effective.

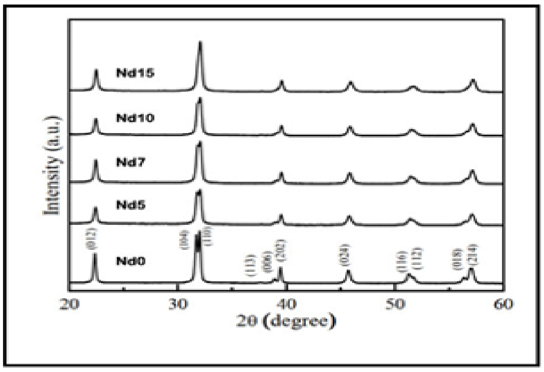

Figure:3 X-ray diffraction patterns for pure and Nd-doped BFO nanoparticles prepared at 450°C.

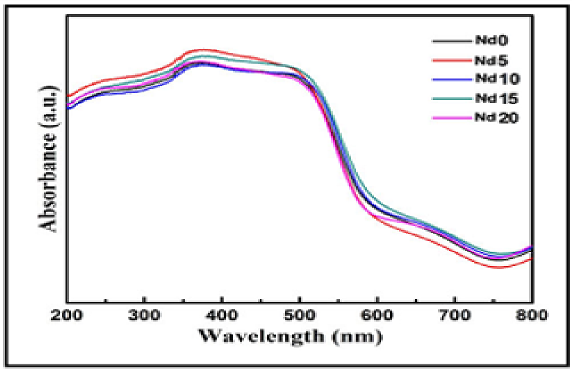

Figure:4 UV–visible Spectrum of for pure and Nd-doped BFO nanoparticles.

Table -1: Percentage degradation efficiencies of undoped and doped BFO on dyes with effect of some parameters like the time, concentration and the source of light

Fact-Finding	**BFO-doped**	**Dosage of catalyst (in g)**	**Degraded Organic dye**	**Initial conc. of dye (mg/L)**	**Light source**	**Time (min)**	**% Degradation**
Chen et al. (2015)	Nd	0.16	Rhodamine B	6.00	300 W Xe lamp	120	59

4. Conclusion:

XRD analysis is a technique used to determine the crystalline structure of a material by analyzing the diffraction patterns of X-rays that are scattered by the atoms within the crystal. The prominent peaks in the XRD plots indicate that the BiFeO3 nanoparticles synthesized are in a pure phase, without any other impurities. UV-visible spectroscopy is a technique used to study the electronic transitions of a material by measuring the absorption of light in the ultraviolet and visible regions of the electromagnetic spectrum. The band gap is the energy difference between the highest occupied energy level (valence band) and the lowest unoccupied energy level (conduction band) in a material, and it determines the material's ability to absorb light and generate electron-hole pairs. The gradual decrease in the band gap from 2.10 eV to 1.98 eV upon doping of Nd indicates that the photocatalytic performance has improved. This improved performance could make them useful in applications such as environmental remediation, where they could be used to degrade organic pollutants in wastewater, or in energy conversion, where they could be used in solar cells to convert light into electricity. The synthesis and characterization of these doped nanoparticles are essential steps in developing efficient and effective photocatalytic materials for all these applications.

Acknowledgement:
Authors are thankful to University Department of Chemistry, Lalit Narayan Mithila University of Darbhanga, Bihar, 846008 India for extending laboratory facility.

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